Applications of Molecular Simulation and Statistical Mechanics

Chemical Engineering 615, Fall 2020 – Times: TTh 11:20-12:40
Location: Duncan Hall - 1046

Instructor: Walter G. Chapman, wgchap@rice.edu, B-241 Abercrombie

This course examines the application of molecular simulation and statistical mechanics to problems of interest to engineers. Topics include simple fluids, molecular fluids, interfaces, ordered systems, and the current literature. A prior course in statistical mechanics is suggested but not required. In the early lectures, the students will learn molecular simulation techniques. Writing and running molecular simulation code provides the students with a "feeling" for the statistical mechanics distribution functions and for the relation between microscopic force models and macroscopic properties. In the latter part of the course the students will work on projects of current research interest while the remaining lectures focus on development of statistical mechanics theory, e.g. perturbation theory, integral equation theory, and density functional theory.

Reference Books:

R.L. Rowley, *Statistical Mechanics for Thermophysical Property Calculations*, PTR Prentice Hall, Englewood Cliffs, New Jersey (1994).

Hansen, J.P. and McDonald, I.R., *Theory of Simple Liquids*, Academic Press, New York.

McQuarrie, D., *Statistical Mechanics*, University Science Books (2000).

Allen, M.P. and Tildesley, D.J., *Computer Simulation of Liquids*, Clarendon Press, Oxford (1987).

Grading will be based on homework (70%) and a final project (30%). Some of the homeworks will be pledged. Grading of the the final project will be based on a paper (66%) and a 15 minute presentation (34%).

Project Presentation dates: Nov. 17 and 19, 2020
Written Project Due: Dec. 16, 2020

Homework assignments will handed out weekly in class. These assignments will be due by 5 PM on the stated due date. Late homeworks will be penalized.

The following topics will be covered in lectures.

I. Atomic Fluids

- Molecular Simulation of atomic systems
  - Metropolis monte carlo simulation in various ensembles
  - Molecular dynamics simulation
- Theory of atomic systems
  - Perturbation theory for atomic systems
  - Integral equation theory for atomic systems

II. Molecular Fluids

- Molecular Simulation for non-spherical systems
- Advanced Simulation Methods
  - Configurational Biased MC
  - Histogram Re-weighting
- Theory for non-spherical systems
  - Integral equation theory (RISM)
  - Perturbation theory

III. Fluids Near an Interface

- Molecular Simulation
- Density Functional Theory

Any student with a disability requiring accommodations in this course is encouraged to contact me after class or in my office. Additionally, students should contact Disability Support Services in the Ley Student Center. Please talk to the Professor if you have any special needs.